Growth of $CuInSe_2$ nanowires by molecular beam epitaxy without external catalyst

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Abstract
Chalcopyrite materials of the composition $Cu(In,Ga)Se_2$ (CIGSe) represent the light absorbing layer in the thin-film solar cell technology with the currently highest power conversion efficiency (21.7% [1]), outperforming multi-crystalline Si solar cells. The most efficient CIGSe material is grown in a three-stage coevaporation process [2]. On the other hand, the use of semiconductor nanostructures has received significant attention in the quest to enhance power conversion efficiencies of solar cells by quantum effects and/or light management structures [3].
We report the growth of $CuInSe_2$ nanowires using a molecular beam epitaxy system where the elemental constituents Cu, In, and Se are evaporated from elemental sources at low evaporation rates of ~0.5 nm/min. The growth of the wires occurs on top of an underlying $CuInSe_2$ polycrystalline layer that initially forms on the Si(100) substrate, where the native oxide has not been removed intentionally. Reference samples, where the native oxide was removed chemically prior to the $CuInSe_2$ growth and where the same growth process is performed, do not exhibit the presence of the nanowires. The structure and composition of single wires were analyzed by transmission electron microscopy (TEM) using selective area electron diffraction (SAED) and energy dispersive x-ray spectroscopy (EDX). The structure of the nanowires is identified as tetragonal, the same structure observed for polycrystalline thin-film material. High resolution (HR) TEM analysis indicates a high crystalline quality of the nanowires. X-ray diffraction (XRD) identifies the polycrystalline layer as $CuInSe_2$ and photoluminescence at low temperature revealed an emission in the range ~0.8-1.0 eV demonstrating strong optical activity of the samples. The visible and near-infrared spectral part of the optical reflectivity of samples with a high density of nanowires is reduced compared to reference samples without nanowires, making the realized nanowire structures interesting for solar energy harvesting. A series of growth experiments with a variation of the growth parameters was carried out to identify a growth model for the $CuInSe_2$ nanowires. Based on the observed relation between nanowire density and growth parameters, we propose the formation of liquid In-Se droplets on the polycrystalline $CuInSe_2$ base layer as a seed for the nanowire growth.

References
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